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# Numerical Simulation of a Low Emissions Gas Turbine Combustor Using KIVA-II

## Part I: Fuel Nozzle/Rich-Burn Zone Analysis

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# NUMERICAL SIMULATION OF A LOW EMISSIONS GAS TURBINE COMBUSTOR USING KIVA-II, PART I: FUEL NOZZLE/RICH-BURN ZONE ANALYSIS

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## ABSTRACT

The use of a staged turbine combustor (STC) for reducing the pollutant emissions is currently under study because it offers a broad operational range due to the good flame stability of the RB zone. A numerical study was performed to investigate chemically reactive flow with sprays inside a STC combustor using a modified version of the KIVA-II code. This STC combustor consists of a fuel nozzle (FN), a rich-burn (RB) zone, a converging connecting section, a quick-quench (QQ) zone, a diverging connecting section, and a lean-combustion (LC) zone. From the computational viewpoint, it is more efficient to split the STC combustor into two subsystems, called FN/RB zone and QQ/LC zones, and the numerical solutions were obtained separately for each subsystem. This paper addresses the numerical results for the FN/RB zone which is equipped with an advanced airblast fuel nozzle. The input conditions used in this study were chosen to be similar to those encountered in advanced combustion systems.

Preliminary results generated illustrate some of the major features of the flow and temperature fields inside the RB combustion zone. From the results obtained so far, it appears that the modified KIVA-II code can be used to study the effects of a number of combustor design and operating parameters, such as fuel split, RB zone geometry, equivalence ratio, etc., on flow and temperature-fields, and pollution emissions.

## INTRODUCTION

The current environmental issue on pollution imposes an urgent need in the reduction of NOx emission from gas turbine engines. One way to reduce the production of NOx from the gas turbine combustor is to utilize the staged turbine combustor (STC) concept (ref. 14). One STC combustor, which consists of a fuel nozzle (FN), a rich-burn (RB) zone, a converging connecting section, a quick-quench (QQ) zone, a diverging connecting section, and a lean-combustion (LC) zone, is shown in figure 1. The STC concept incorporates staged burning. Combustion is initiated in the RB zone with an equivalence ratio ($\phi$) in the range of 1.2 to 2.0. The hydrocarbon reactions proceed rapidly, depleting the available oxygen, thereby inhibiting NOx formation. The hot rich mixture is then rapidly diluted and mixed by an array of air dilution holes or slots in the QQ zone. The combustion is completed with $\phi$ in the range of 0.4 to 0.6 stoichiometric in the LC zone. The STC concept offers a broad operational range because of the good flame stability of the RB zone. It is also known that one key element for successful reduction of NOx from the exhaust of STC combustors is the proper design of dilution jet mixing in the QQ zone. Therefore, to increase the performance efficiency and to reduce the NOx pollutant emissions, the mixing process becomes essential to the design of STC combustors.

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There are several approaches that can be used to numerically solve the chemically reactive fluid flow and heat transfer occurring inside the STC combustor shown in figure 1. One is to consider the whole combustor as a single unit. Another is to isolate each zone with the interrelations between zone treated through the inlet/outlet boundary conditions. For instance, the outlet condition of the RB zone can be used as the inlet condition of the QQ zone. This allows the zones to be treated differently. For example, the RB zone can be assumed to be axisymmetric (with swirl) while the QQ zone must be considered to be three-dimensional due to the discrete slots. Therefore, for computational efficiency, the RB zone was calculated as an axisymmetric problem with a finer mesh to resolve the airblast nozzle passages. The QQ zone was calculated as a three-dimensional problem using a coarser sector mesh to isolate one slot. In order to minimize the effect of the interzone boundary conditions, the zones had a considerable amount of overlap.

The purpose of this two-part paper is to present a multidimensional numerical analysis of the turbulent two-phase reacting flows inside the STC combustor. An advanced airblast nozzle was used as a means of supplying air and fuel for the RB zone. The geometry of the fuel nozzle is shown in figure 2. The nozzle has two fuel injection passages and four air flow passages. The inner flow passage has a counter-rotating swirler with 63° van angle. The van angles of the middle, outer, and dome flow passages are 61.3°, 60.2°, and 60.2°, respectively, and are all co-rotating. In the QQ zone, cool dilution air is injected into the hot rich mixture through inclined slots. This paper is concerned with the numerical analysis of the FN/RB zone. The QQ/LC zones solutions are given in a second paper. Figure 3 shows the FN/RB zone and the QQ/LC zones computational sections.

Computational fluid dynamics (CFD) has been used to model simple gas turbine combustor flow fields for the past decade. The predicted results of many of these studies (refs. 5 to 8) showed a lack of agreement with experimental data due to excessive numerical diffusion, inaccurate turbulence models and inlet boundary specifications, and inaccurate grid and coordinate systems used. The most recent studies dealing with the QQ zone dilution jet mixing problems in flametube combustors can be found in references 9 to 12. In their studies, the effects of momentum flux ratio and mixing flow area on mixing were investigated by using a simplified quick mixer geometry. They reported that, for better mixing, the residence time at high flame temperatures should be reduced and that there are optimum values of momentum flux ratio and slot aspect ratio (refs. 9 to 10). This paper reports the use of an advanced CFD code, KIVA-II (refs. 13), to analyze a potential complex STC combustor.

## DESCRIPTION OF PROBLEM

Since the flow field in FN/RB zone is essentially axisymmetric, only one axial- radial plane of computational cells was considered. Accordingly, the system under investigation is shown in figure 4 in which D is the diameter of the QQ zone and $L_{rich}$ is the length of the RN zone. It is noted that, to avoid flow contamination due to inlet/outlet boundary conditions, the outlet boundary of the FN/RB zone was extended to the end of the convergence section.

The following inlet conditions were chosen:

Temperature = 1000 °F (811 K)
Pressure = 90 psia ($6.205\times10^6$ dynes/cm$^2$)
Air mass flow rate = 1.09 lbm/sec (494.42 g/s)
Air flow split = 7.8/19.1/25.5/47.6 percent (from inner to dome)
Air flow passage area = 0.007/0.0117/0.0156/0.027 ft$^2$ (6.50/10.87/14.49/25.08 cm$^2$)
Equivalence ratio = 1.4
Fuel split = 50/50 percent
Turbulent length scale = 0.25 of the respective flow passage width
Turbulent kinetic energy = 1 percent of the respective 0.5 $W^2$

where W is the mean axial velocity at inlet.

The inlet boundary conditions were the specification of the density (calculated from the temperature and pressure given above) and W (calculated from the mass flow rates and flow areas given above). The radial velocity component was set so that the inlet flow was tangent to the flow passages. The azimuthal or swirl velocity component was specified assuming wheel flow. The turbulent kinetic energy and length scale were specified at the values given above. The exit boundary condition was a specified exit pressure. Since this pressure is coupled with the QQ/LC zones inlet condition due to the flow is subsonic, an iteration procedure is therefore needed to update the FN/RB zone outlet pressure as described in the second part of this paper (ref. 14). The combustor walls were assumed to be adiabatic with a turbulent boundary layer. These conditions were enforced using wall functions (ref. 13).

## NUMERICAL METHOD OF SOLUTION

The numerical solutions were obtained using a modified version of KIVA-II, implemented to study the aforementioned objective. The grid system (81×51 grid points) needed for the solution was generated by an algebraic/elliptic method and is shown in figure 5.

### The KIVA-II Code

The KIVA-II code (ref. 13) developed at the Los Alamos National Laboratory is an advanced computer program for the numerical calculation of transient, two- and three-dimensional, chemically reactive fluid flows with sprays. It solves the unsteady equations of motion of a turbulent, chemically reactive mixture of ideal gases, coupled to the equations for a single-component vaporizing fuel spray. The numerical scheme is based on the arbitrary Lagrangian-Eulerian (ALE) method (refs. 15 and 16) with implicit continuous Eulerian modification for low Mach number flows. A stochastic particle method is used to calculate the evaporation rate of liquid sprays. The effects of droplet oscillation, distortion, breakup, collision, and coalescence are considered in the computations. Several upwind convection schemes, such as the partial donor cell and quasi-second-order upwind, are included. Two turbulence models, modified $\kappa$-$\varepsilon$ and subgrid scale models, are also available. For additional details of the KIVA-II, see reference 13.

### Code Modifications

Since the KIVA-II is primarily written for solving the reciprocating internal combustion engine problems, modifications are needed for the application to the current problem. Following are the descriptions of the major changes made to the code.

The fuel was considered as Jet-A in the liquid phase and propane in the gas phase, according to Nguyen and Ying (ref. 17). The propane combustion was modeled using a simplified 11-reaction set (five kinetic reactions and six equilibrium reactions). The five kinetic reactions are:

$$C_3H_8 + (3/2 + 8/4)\,O_2 \leftrightarrow 3\,CO + 4\,H_2O$$
$$CO + 1/2\,O_2 \leftrightarrow CO_2$$
$$O + N_2 \leftrightarrow N + NO$$
$$O_2 + N \leftrightarrow O + NO$$
$$N + OH \leftrightarrow H + NO$$

and the six equilibrium reactions are (ref. 18):

$$H_2 \leftrightarrow 2\,H$$
$$O_2 \leftrightarrow 2\,O$$
$$N_2 \leftrightarrow 2\,N$$
$$O_2 + H_2 \leftrightarrow 2\,OH$$
$$O_2 + 2\,H_2O \leftrightarrow 4\,OH$$
$$O_2 + 2\,CO \leftrightarrow 2\,CO_2$$

Details of this simplified chemical reaction model together with the reaction constants can be found in reference 17.

The grid system was generated separately and KIVA-II was modified to read the grid information accordingly. The geometry routines were modified to allow four separate inlet flow passages to be defined. The boundary condition routines were modified to allow separate inlet conditions for each passage. In addition, the boundary condition routines were modified to allow arbitrary shaped combustor walls. Properties of Jet-A liquid fuel were also added to the code.

Species information both at the inflow and fuel sprays were specified and the necessary modifications were made to include the number of species and their thermodynamic properties. Calculations of the emission index of CO and NO were also included. The emission index was defined as a ratio of the grams of pollutant formed divided by the kilograms of fuel consumed.

## RESULTS AND DISCUSSION

Preliminary results were obtained using the quasi-second-order upwind scheme in the KIVA-II code. In the calculation of spray droplets, only the evaporation submodel was used.

To closely simulate a real engine operating procedure, the code was executed as follows. At the beginning, the fuel sprays and ignition were turned off, and the program was run with air only for 1,000 time steps, which corresponds to 18.871 millisecond (ms) real time simulation. The flow field after 1,000 time steps is shown in figure 6, with the streamlines superimposed on the velocity vectors. Figure 7 shows the enlarged view of the velocity field near the inlet. The two recirculation zones, one located near the center-line and the other at the left upper corner, are typical to the combustor geometry under study. The size and shape of the center-line recirculation zone has an important influence on the performance of the RB zone.

Starting from the cold flow simulation, the code was restarted with both fuel injectors and ignitor turned on at 18.872 ms. The ignitor was turned on for 1 ms and the location of the ignition window is shown in the crosshatched area in figure 5. The reciprocal time constant for ignition energy addition to the ignition cells was set to $2.61\times10^3$ in the KIVA-II input file. Figure 8 shows the flow, pressure, and temperature fields at 21.443 ms (1,200 time steps). There is a higher temperature region, isotherm levels 2 to A, near the ignitor, indicating where the chemical reaction is taking place. Due to the chemical reactions, high pressure waves are created and are propagating downstream causing the center-line recirculation zone to disappear temporally. It can be seen clearly that the lower temperature region, enclosed by the isotherm level 1 envelope is basically made up of the fuel rich mixture (the inlet temperature of fuel at the injectors was 293 K and the inlet air temperature was 811 K). Figure 9 gives the distribution of the liquid fuel particles. The interface of isotherm levels 1 and 2 in figure 8 is the location where the fuel rich mixture encountered the high temperature flame front.

Figure 10 shows the flow and temperature fields at 25.469 ms (1,600 time steps). From this figure, it is observed that the center-line recirculation zone is recovering and the high temperature regions are gradually convecting downstream. There is a high temperature gradient building up near the interface of isotherms 1 and 2. The size of level 1 envelope at this instant is a bit larger than the one shown in figure 8, an indication of the fuel vaporization.

Figures 11 and 12 show the flow, pressure, and temperature fields and the liquid fuel particle distribution at 108.98 ms (9,000 time steps) and 120.3 ms (10,000 time steps), respectively. It can be seen that the solution has reached steady state at 120.3 ms. The emission index of CO and NO, calculated at the locations indicated by stars in figure 5, is given in figure 13.

For the purpose of comparison, figure 14 gives the flow field under pure flow condition, i.e., without fuel spray and chemical reaction. As one can see, without chemical reaction, the center-line recirculation zone is very large. Results obtained from this part will be used as the inlet condition for the second part of this study.

## CONCLUSIONS

Modification of KIVA-II for the study of STC combustor FN/RB zone with an advanced airblast nozzle has been completed. Preliminary results from the application of this modified version of KIVA-II to the study of the chemically reactive flows inside the FN/RB zone show some of the major features of the flow and temperature fields inside the rich combustion zone. From the results obtained so far, it appears that the modified code can be used to study the effects of a number of combustor design and operating parameters, such as the fuel split, air flow split, RB zone geometry, equivalence ratio, etc., on flow, temperature, and pollution emissions.

## ACKNOWLEDGMENTS

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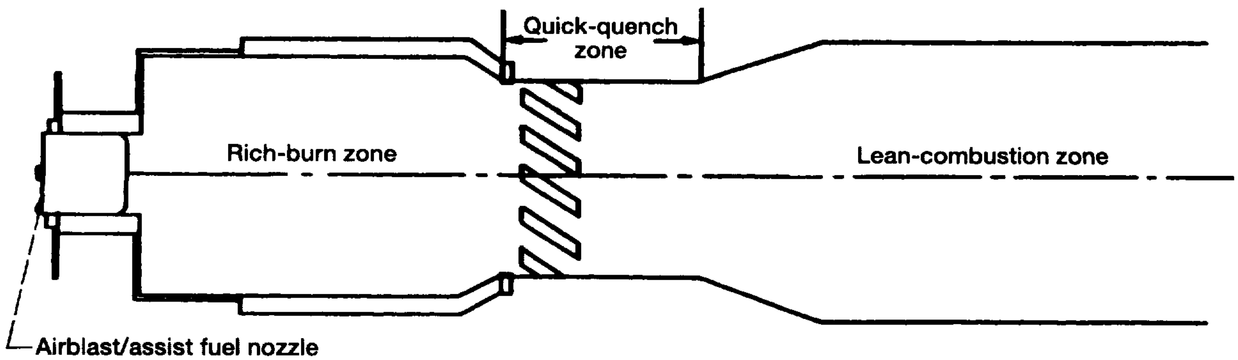

Figure 1.—Schematic of a staged turbine combustion.

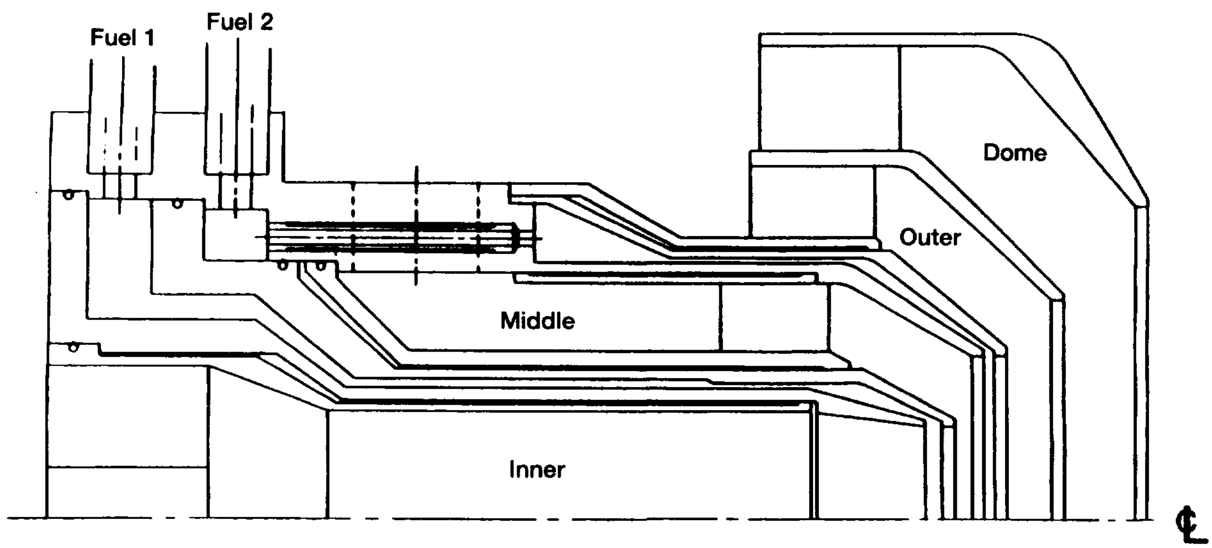

Figure 2.—Schematic of an advanced airblast nozzle.

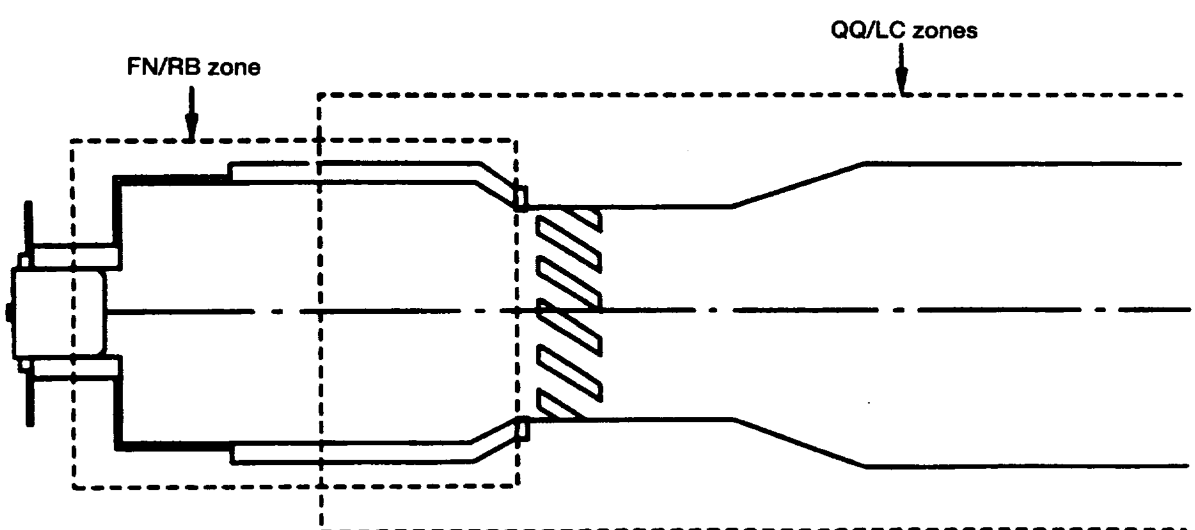

Figure 3.—FN/RB zone and QQ/LC zones computational sections.

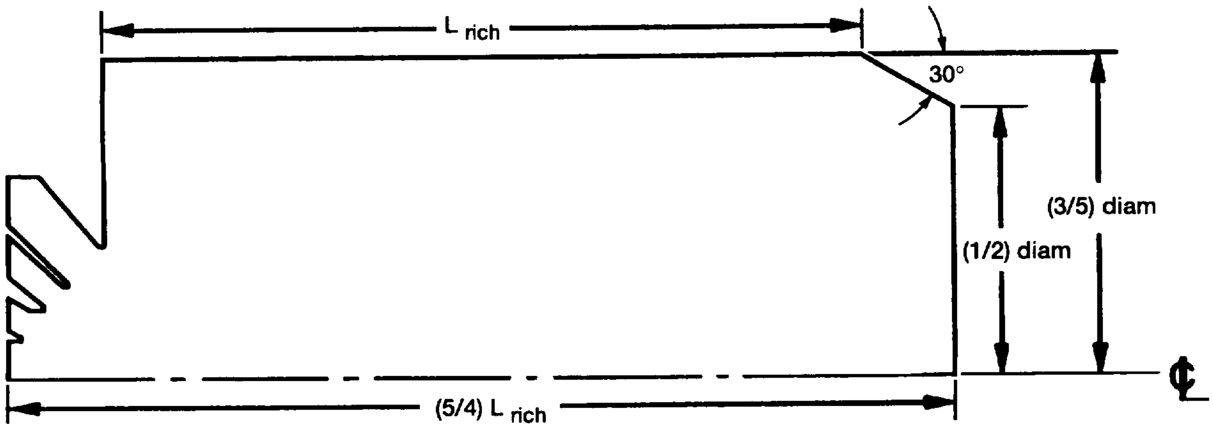


Figure 4.—Geometry of the system under investigation and it's specifications.

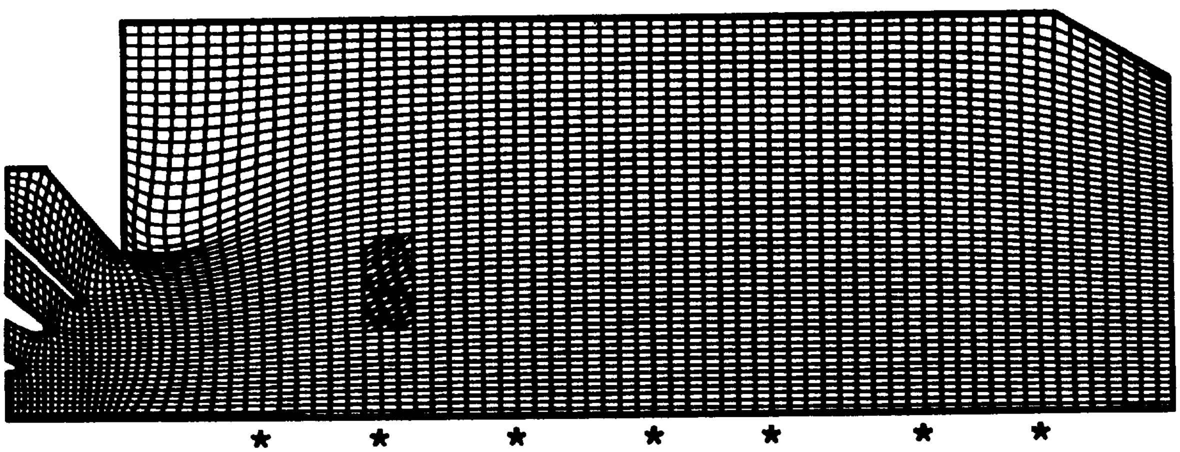

Figure 5.—FN/RB zone computational mesh.

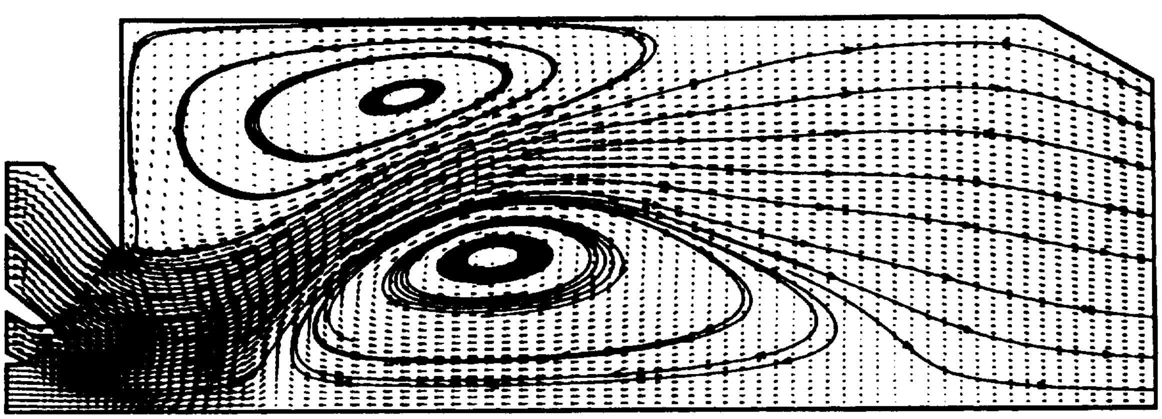

Figure 6.—Velocity vectors and streamlines at t = 18.871 ms.

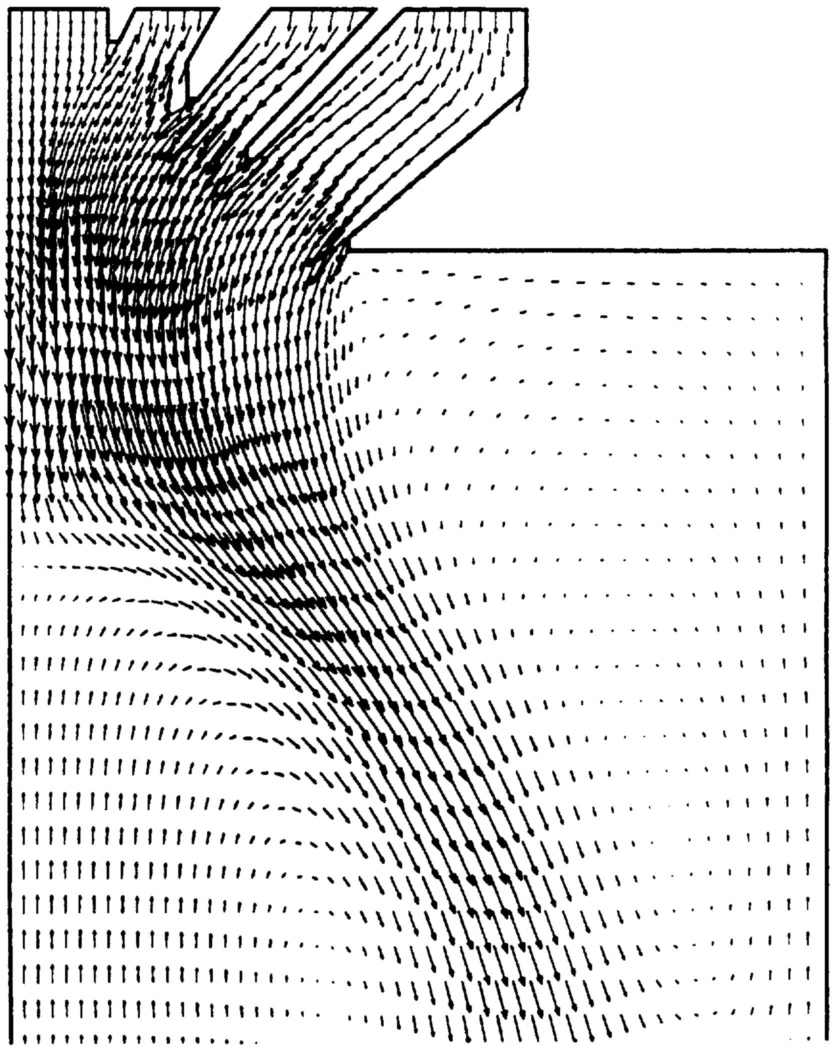

Figure 7.—Enlarged view of velocity vectors near the inlet.

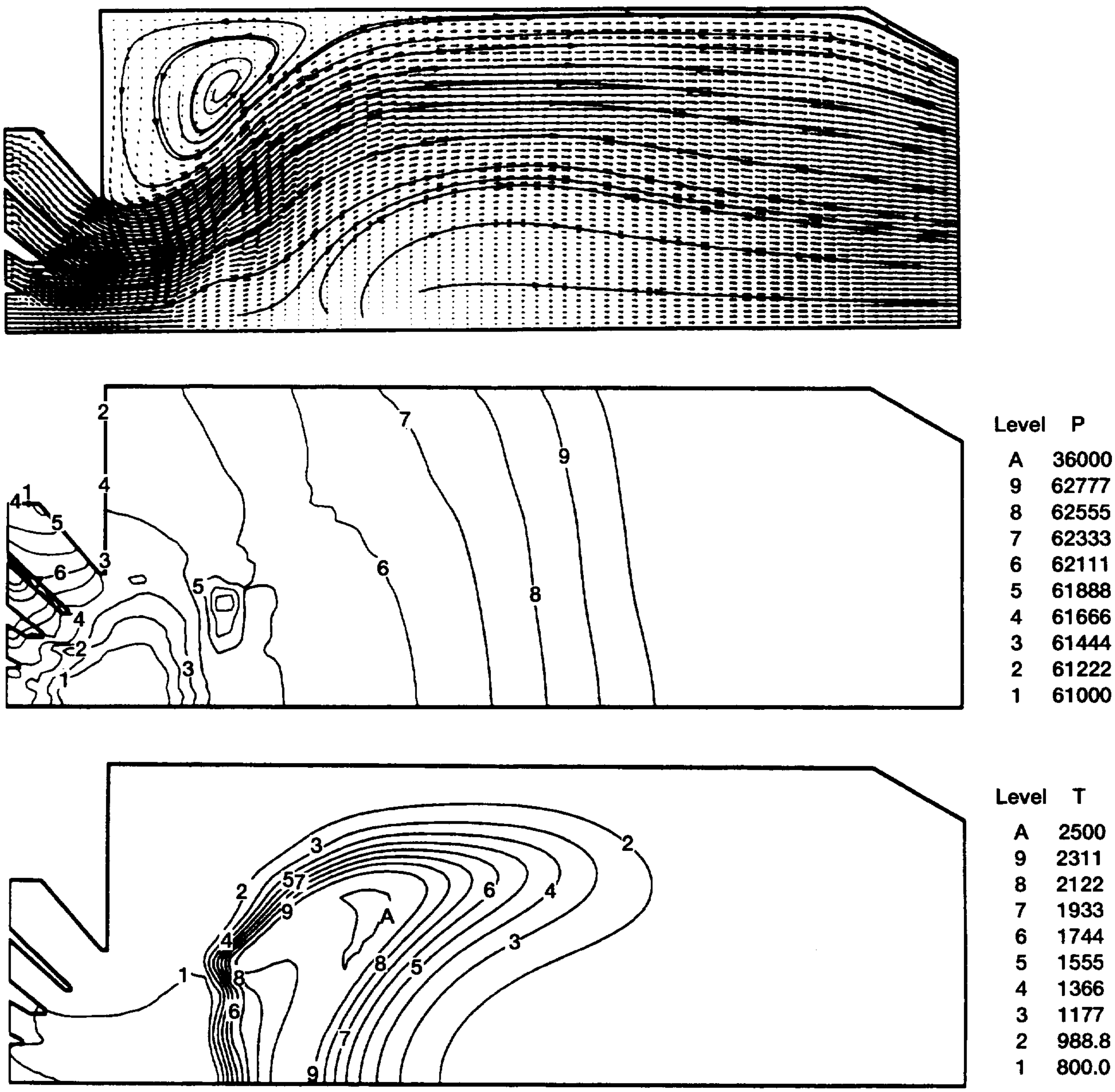


Figure 8.—Velocity, pressure, and temperature fields at t = 21.443 ms.

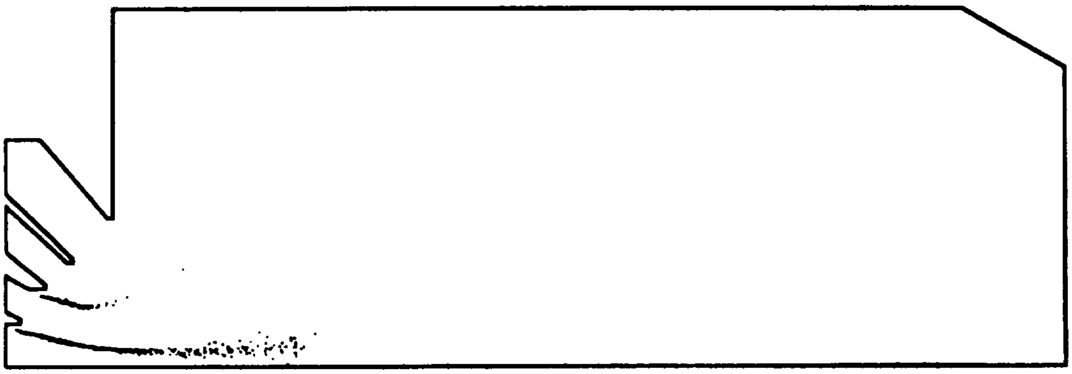

Figure 9.—Distribution of the liquid fuel particles.

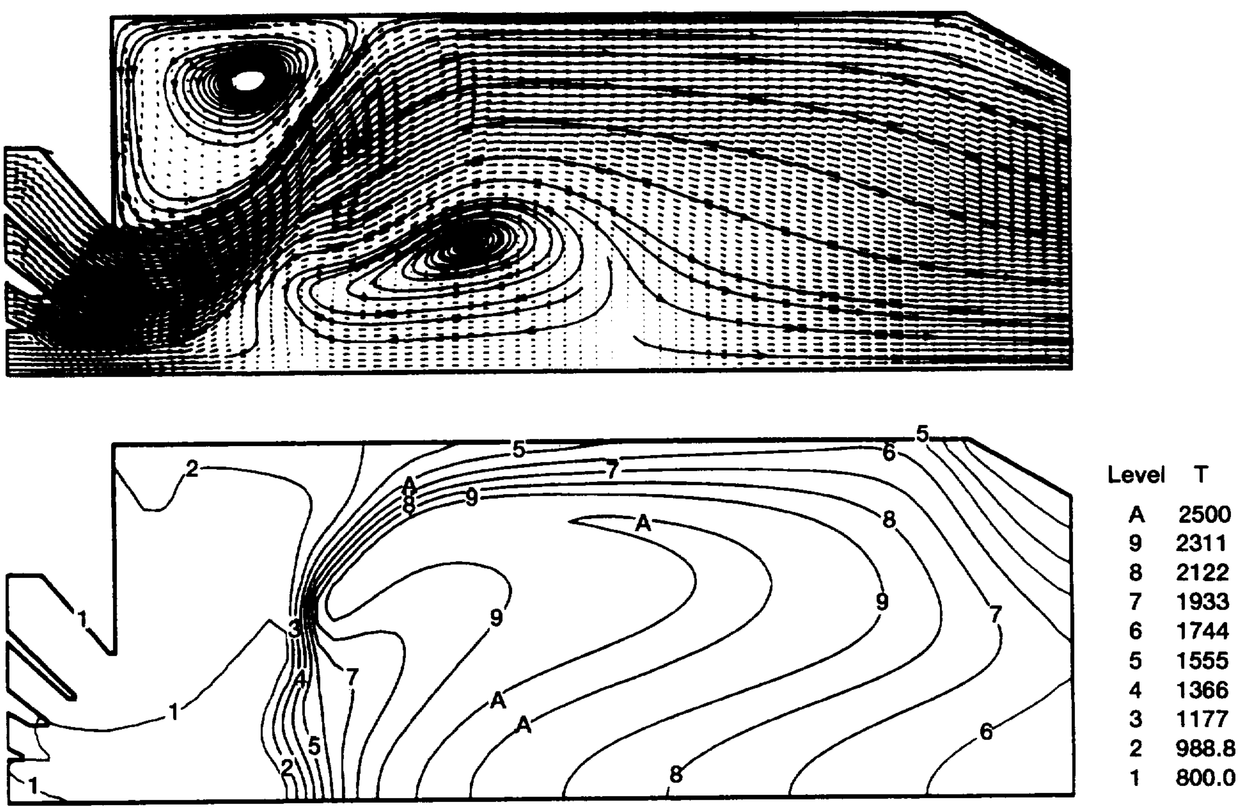


Figure 10.—Flow and temperature fields at t = 25.469 ms.

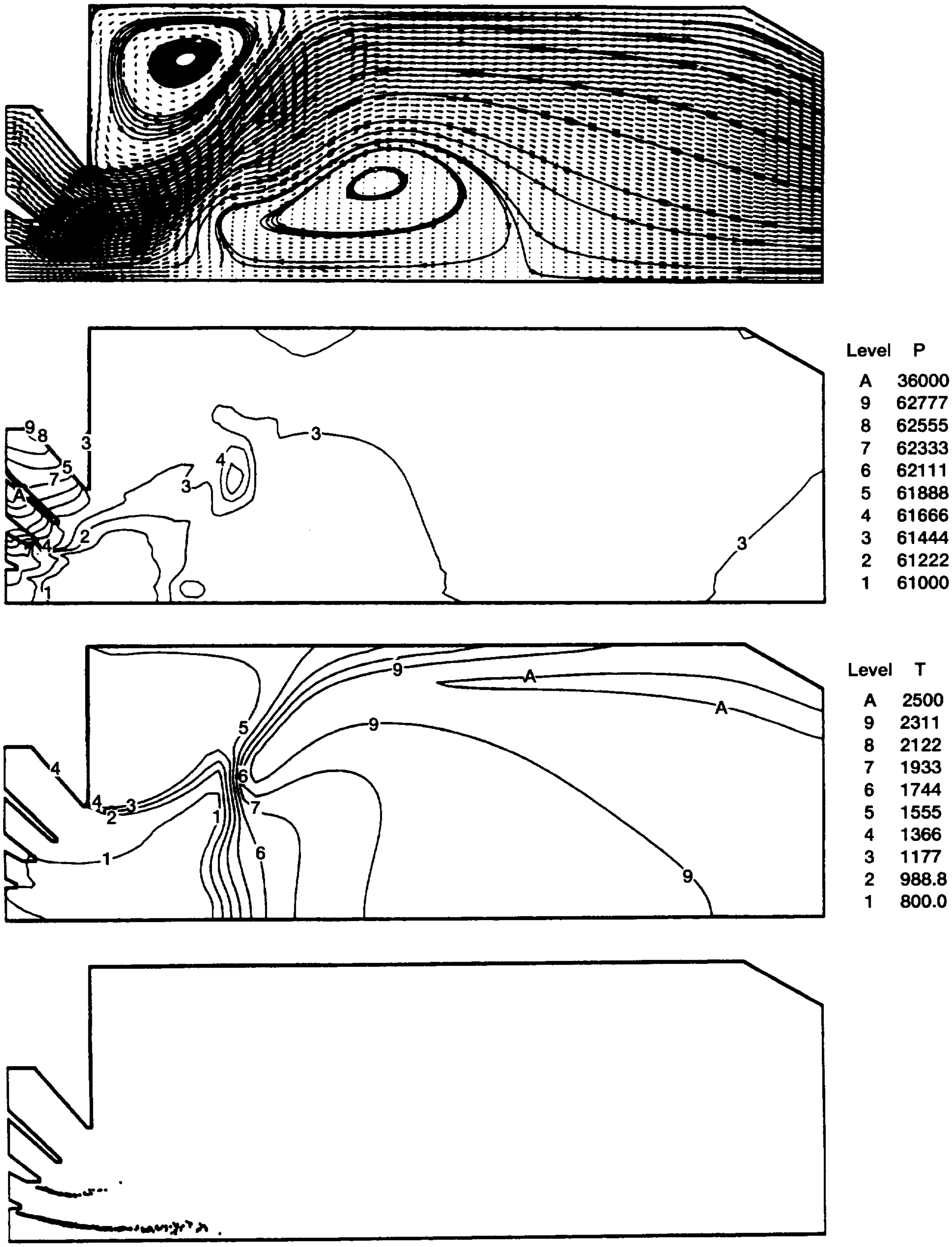


Figure 11.—Velocity, pressure, and temperature fields and the liquid fuel particles at t = 108.98 ms.

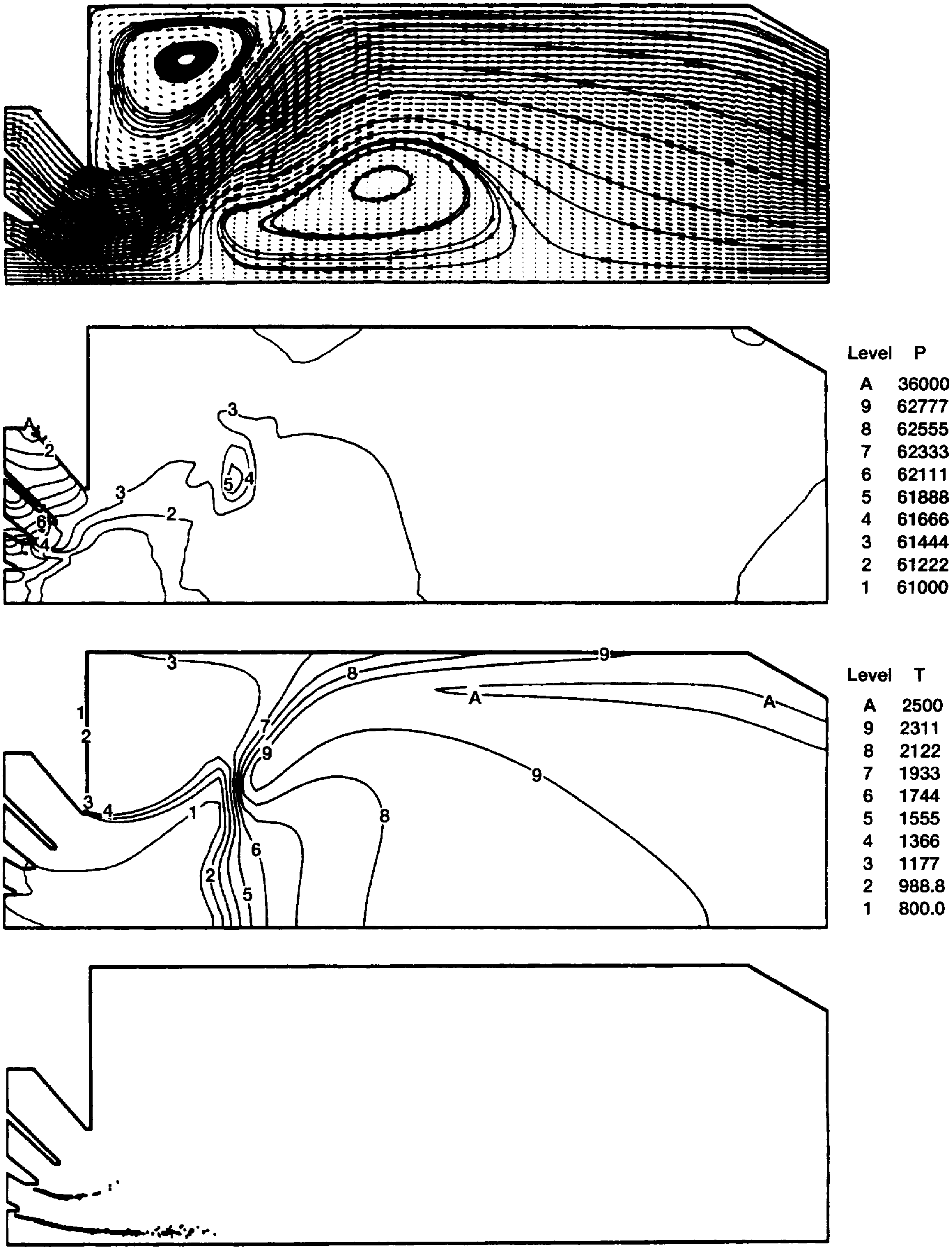


Figure 12.—Velocity, pressure, and temperature fields and the liquid fuel particles at t = 120.3 ms.

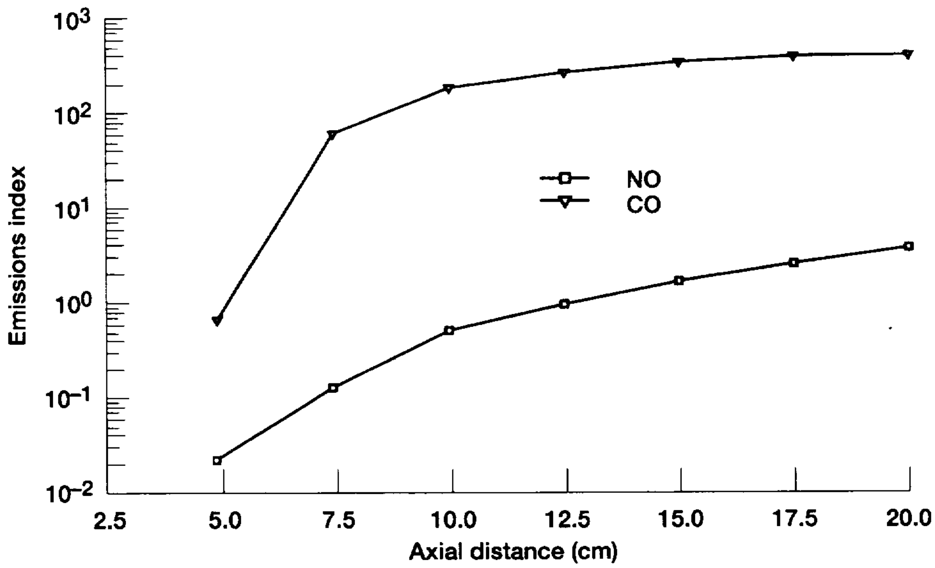


Figure 13.—Emission index of CO and NO.

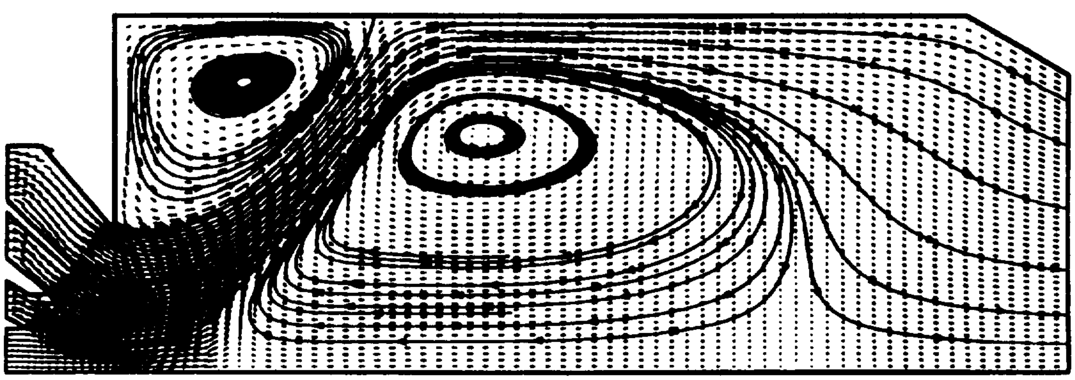

Figure 14.—Pure flow velocity vectors.

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